# Infrastructure and Services Enabling Academic Research

## NITRD MAGIC Team Meeting, Feb-5-2014

*John McGee, and the RENCI ACIS Team*

renci

RESEARCH \ ENGAGEMENT \ INNOVATION

# Today's Agenda

- RENCI architecture and support for High Performance Clusters, including, storage, data, compute, identity management,…
- Lots of details about hardware and software, with some lessons learned
- Discussion of a few research projects and how they build on top this CyberInfrastructure

# About RENCI

- An applied research institute of UNC-CH
- We partner with UNC Research Computing on many initiatives
- Our board is comprised of the CROs and Provosts from NC State, Duke, and UNC-CH
- Build new collaborations and accelerate research activities spanning the three universities
- Develop new Cyberinfrastructure capabilities
- Host leading edge services and platforms for research

# RENCI's ACIS Team

## Casey Averill

VMWare, StorNext, AD, Exchange
SQL Server; 90%

## Mark Montazer

Data center facilities, cooling, UPS, generator, purchasing, end user support for RENCI; 100%

## John McGee

Vision, team lead, team advocate, administrivia; 25%

## Marcin Sliwowski

Sr. Linux admin, storage, clusters, 80%

## Jonathan Mills

Sr. Linux admin, clusters, master puppeteer; 50%

## We are hiring!!

Linux admin, cloud technology (ACIS, ExoGENI)
https://unc.peopleadmin.com/postings/35013

Everyone works on (almost) everything, topics listed are areas of leadership

# Locations where RENCI operates equipment

EDC

GSB

GSC

MDC

| | | |
|---|---|---|
| EDC | Europa Data Center | RENCI Main location |
| MDC | Manning Data Center | UNC Central IT, Research Computing |
| GSB | Genome Sciences Building | UNC School of Medicine |
| GSC | Galapagos Science Center | UNC Center for Galapagos Studies |

# Europa Data Center: Facilities

- 2000 square feet of floor space on an 18 inch raised floor

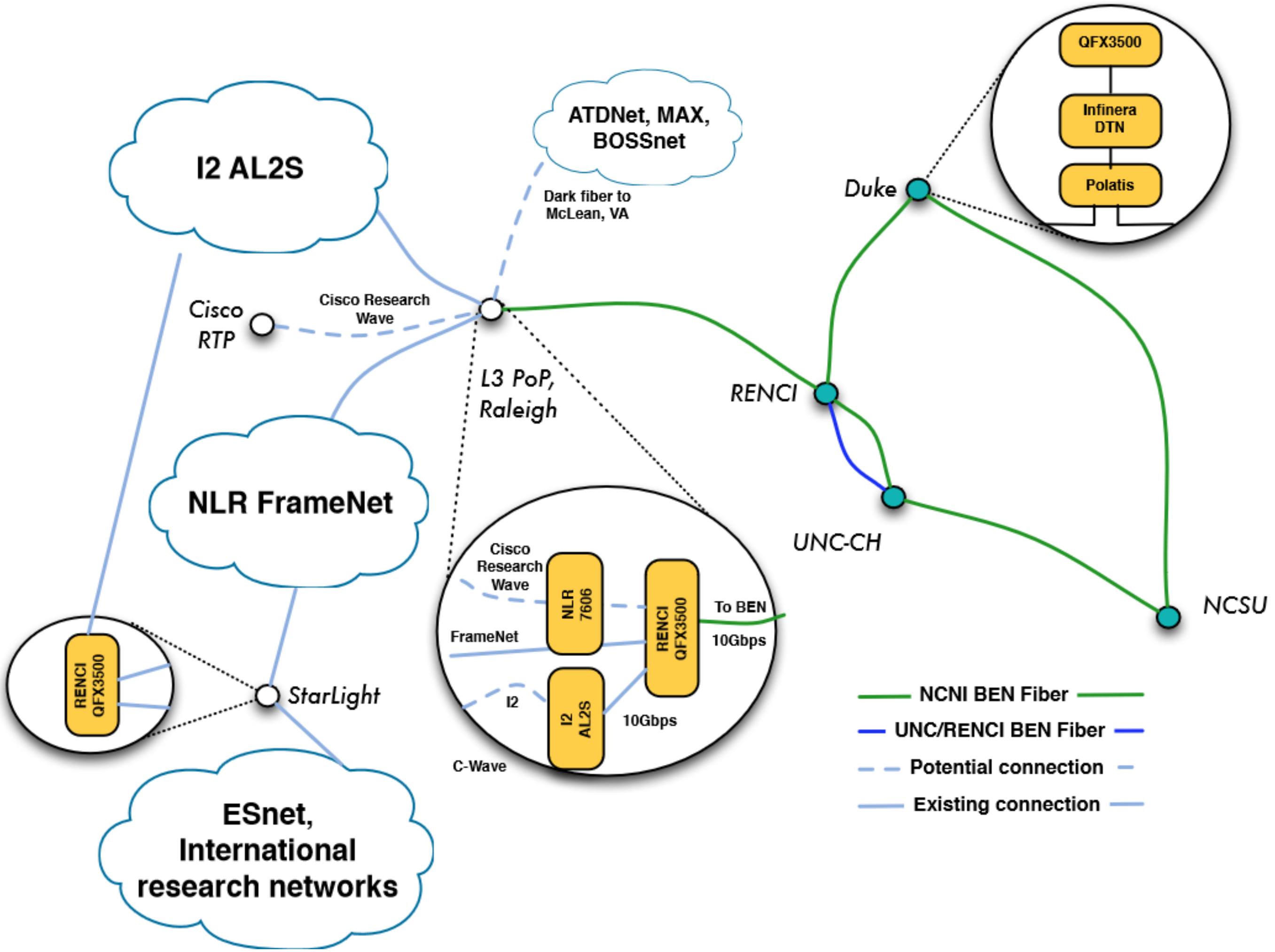
- 600 kva commercial power
- 375 kva UPS power
- 20 kva generator power

- 134 tons dedicated cooling

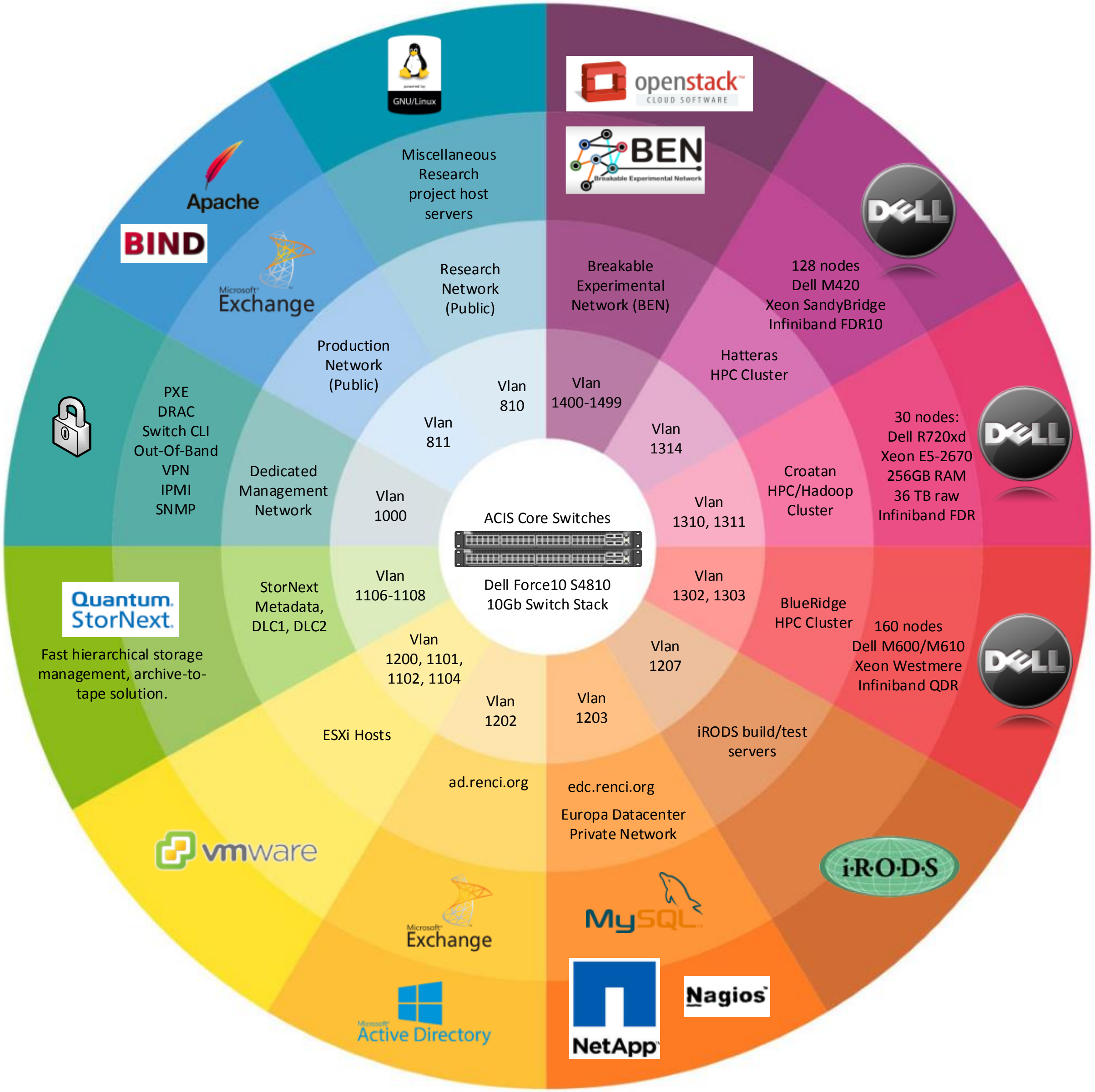
- Room for 40 Racks

EDC: RENCI's main location

# Network Overview



# Extensive use of vlans



ACIS Core Switches

Dell Force10 S4810
10Gb Switch Stack

Vlan
810

Research
Network
(Public)

Miscellaneous
Research
project host
servers

Vlan
811

Production
Network
(Public)

Vlan
1000

Dedicated
Management
Network

PXE
DRAC
Switch CLI
Out-Of-Band
VPN
IPMI
SNMP

Vlan
1106-1108

StorNext
Metadata,
DLC1, DLC2

Fast hierarchical storage management, archive-to-tape solution.

Vlan
1200, 1101,
1102, 1104

ESXi Hosts

Vlan
1202

ad.renci.org

Vlan
1203

edc.renci.org

Europa Datacenter
Private Network

Vlan
1207

iRODS build/test
servers

Vlan
1302, 1303

BlueRidge
HPC Cluster

160 nodes
Dell M600/M610
Xeon Westmere
Infiniband QDR

Vlan
1310, 1311

Croatan
HPC/Hadoop
Cluster

30 nodes:
Dell R720xd
Xeon E5-2670
256GB RAM
36 TB raw
Infiniband FDR

Vlan
1314

Hatteras
HPC Cluster

128 nodes
Dell M420
Xeon SandyBridge
Infiniband FDR10

Vlan
1400-1499

Breakable
Experimental
Network (BEN)

# Storage Strategy

- Highly diverse set of requirements, both in terms of performance characteristics, and in connectivity mechanics, eg: Fiber Channel, iSCSI, NAS

- Compute and data analytics clusters
- Bulk transfers to/from other data centers
- Underlying capabilities for iRODS data grids
- Archive, for some definition of the word
- Genomics, Environmental Science, National Collaborations

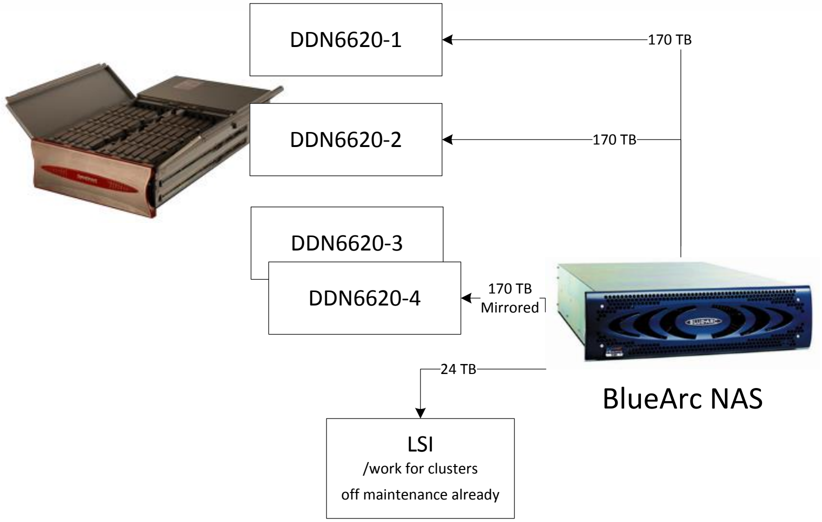
- We optimize for flexibility
- Minimize the human cost of enterprise storage management

# Storage: Current Generation

1. NetApp FAS – research; 1.1PB
2. NatApp FAS – production; 50TB
3. NetApp FAS – MDC 1.5PB (March-2014)
4. Quantum StorNext; 2 - 3.5PB
5. Kaminario all flash array; 6TB

6. Croatan Data Analytics Cluster; 1PB
7. Individual Project Servers w/ Direct Attached Storage; varies
8. Winding down: DDN and BlueArc; 1.1PB

# Storage: Prior Generation


DDN6620-1

DDN6620-2

DDN6620-3

DDN6620-4

LSI
/work for clusters
off maintenance already

BlueArc NAS

Network Attached Storage

DDN9900

Block storage only. Direct attached to various servers or VMs

Multi-vendor solution was complex

Numerous issues with DDN support and controller firmware

BlueArc was purchased by Hitachi during the lifetime of this deployment

Cannot operate these systems without vendor maintenance agreements

The geek in our soul would like to try low cost hardware with open source systems

# Storage: Primary Research Storage (NAS, SAN)

NetApp Clustered Data ONTAP

2 x (FAS6620 Controller, 3TB FlashCache)

8 x (Disk shelves, each with 48 x 3TB drives)

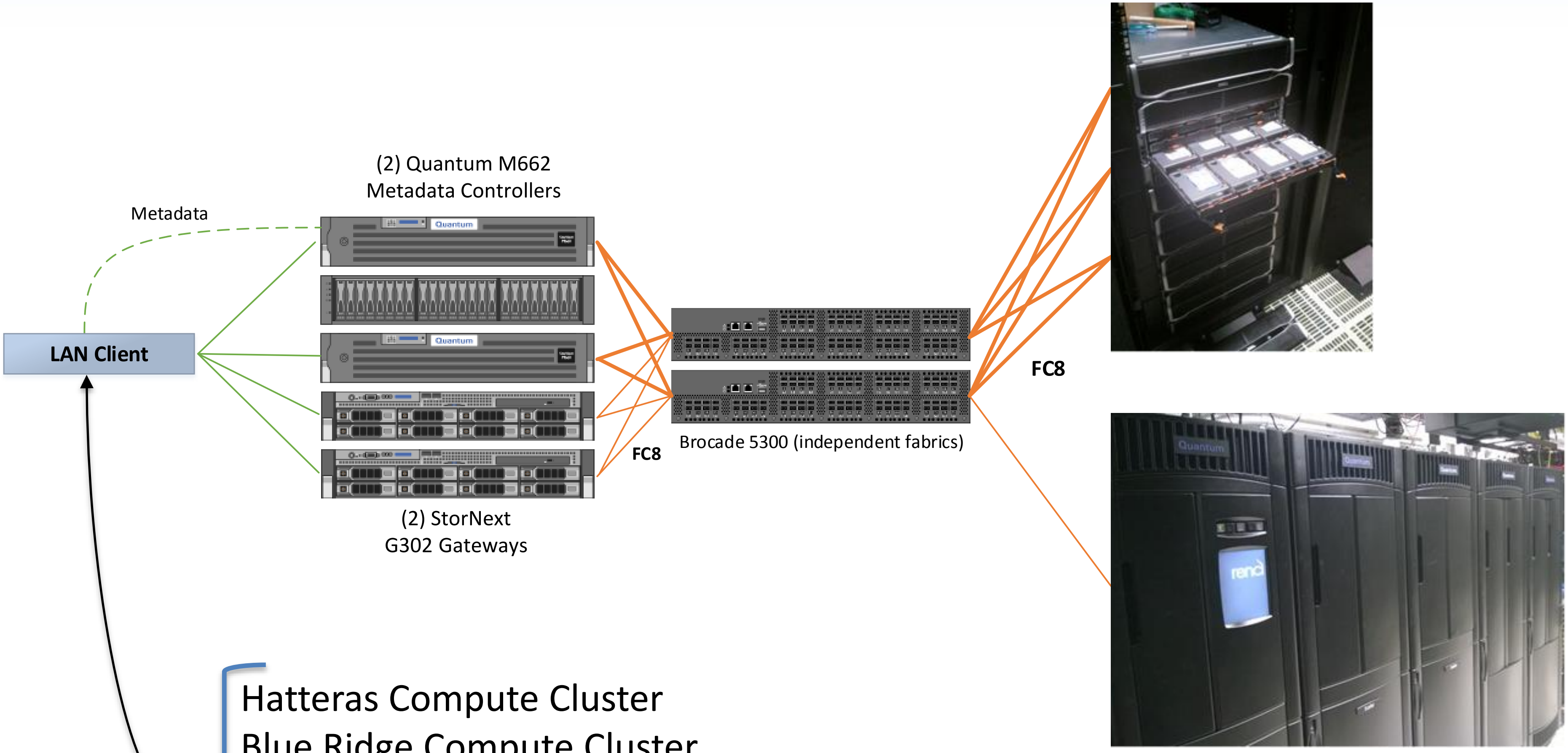
8 x FC8 connections

8 x 10GbE connections

Hatteras Compute Cluster
Blue Ridge Compute Cluster
Croatan Data Analytics Cluster
VMs in the VMWare farm
Project Specific Servers

# Storage: StorNext, secondary research storage + archive

**528TB**:  (8) Dell MD3660f; each with 5 shelves
each shelf has: (1) 400GB SSD, (11) 1.2TB 10k disks



**1.5 to 3 PB**:  Quantum i6000

Hatteras Compute Cluster
Blue Ridge Compute Cluster
Croatan Data Analytics Cluster
VMs in the VMWare farm
Project Specific Servers

# Storage: Experimental System

Kaminario 6TB all flash array

Evaluated performance with VMWare (see link below)
ExoGENI: tested as an iSCSI device for rapid VM provisioning
Relational Database for Genomics processing

http://www.hpcwire.com/off-the-wire/kaminario-renci-announce-report-storage-hpvcs/

# CI-BER: CI for Billions of Electronic Records

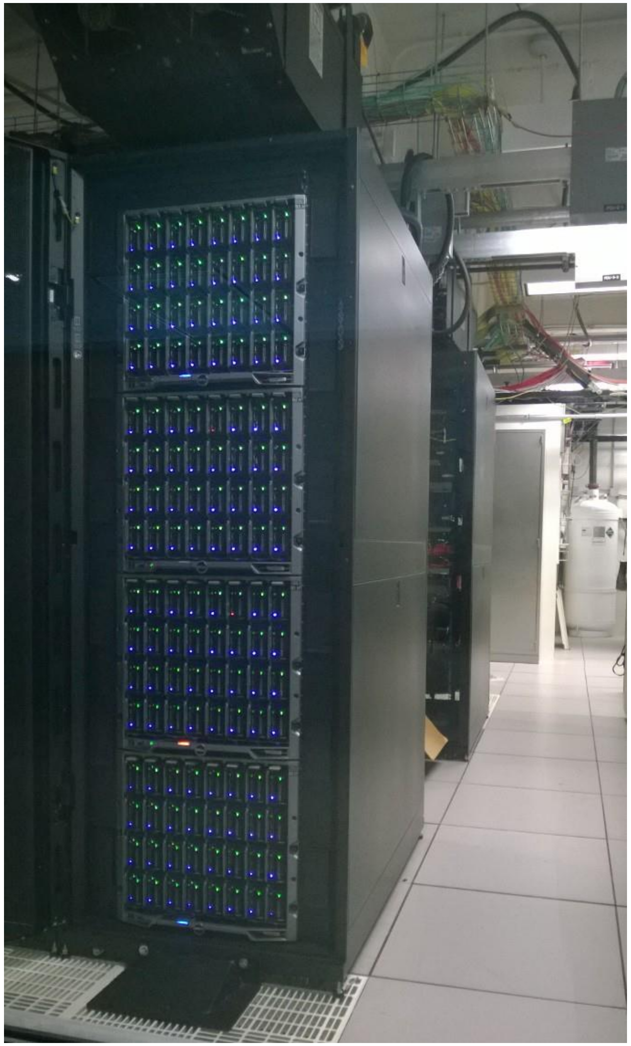
- Approximately: 105TB, 150 million files

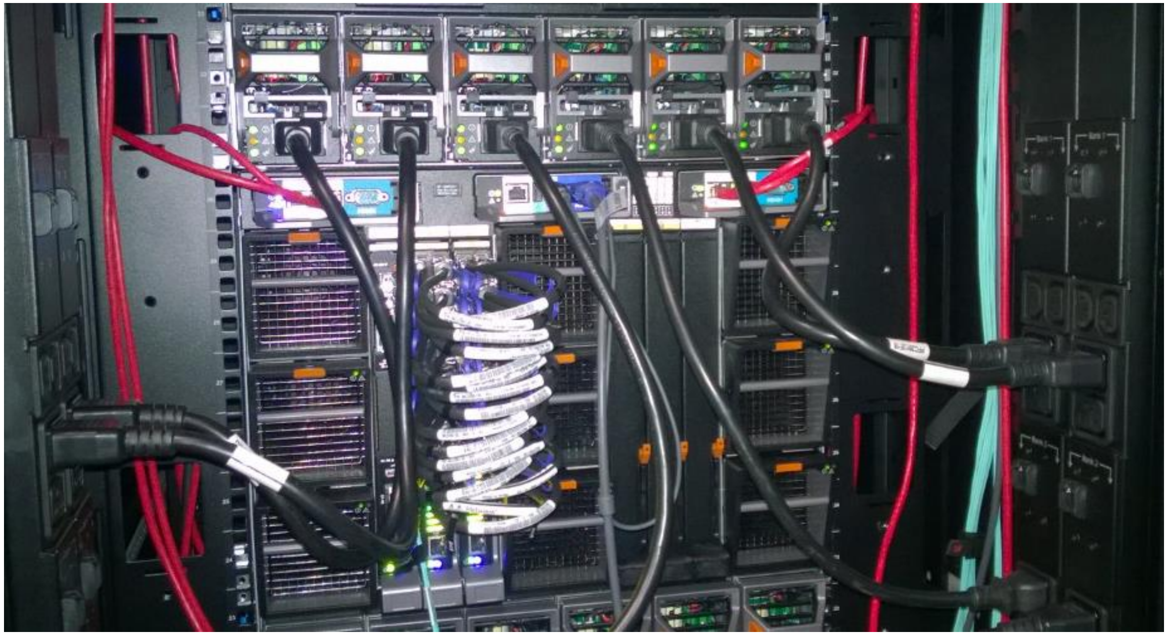
- Capacity is not unruly by our norm, however the file count has proven to be an interesting experience
- Migrating out of the shared infrastructure and onto a dedicated storage system
- Front-end services (iRODS) remain as VMs in the farm

http://sils.unc.edu/news/2012/ci-ber-big-data

# Compute: Hatteras Cluster

- Designed for HPC ensembles
- 4 x (512 cores with 6GB per core; packaged in 32 nodes)
- 40Gb FDR-10 Infiniband Interconnect
- 20GbE uplink per M1000e to storage/rest of the world
- Chose Not to purchase and manage the interconnect to enable MPI across the boundaries of the four 512 core units
- Fits into a single rack
- First RENCI resource to use SLURM





# Compute: Blue Ridge Cluster

- 160 nodes: each with 8 cores, 3GB per core
- 40gb Infiniband interconnect

- 2 GPGPU nodes: 96GB ram, nVidia Tesla S1070
- 2 LargeMem nodes: 32 cores, 1TB ram

- Includes nodes dedicated to a specific project (ADCIRC)

- 10 nodes of similar hardware configuration running Windows HPC

# Data Analytics: Croatan Cluster

- 30 x (Dell R720xd), *each* with:
  - 16 cores at 3Ghz
  - 256GB memory
  - 36TB direct attached storage
  - 56Gbps FDR Infiniband and 40Gbps Ethernet interconnect
  - 10GbE Dedicated NAS Connectivity
  - 1GbE management network
- Aggregate: 1PB raw storage, 7.6TB ram

# Virtual Machine demand has skyrocketed

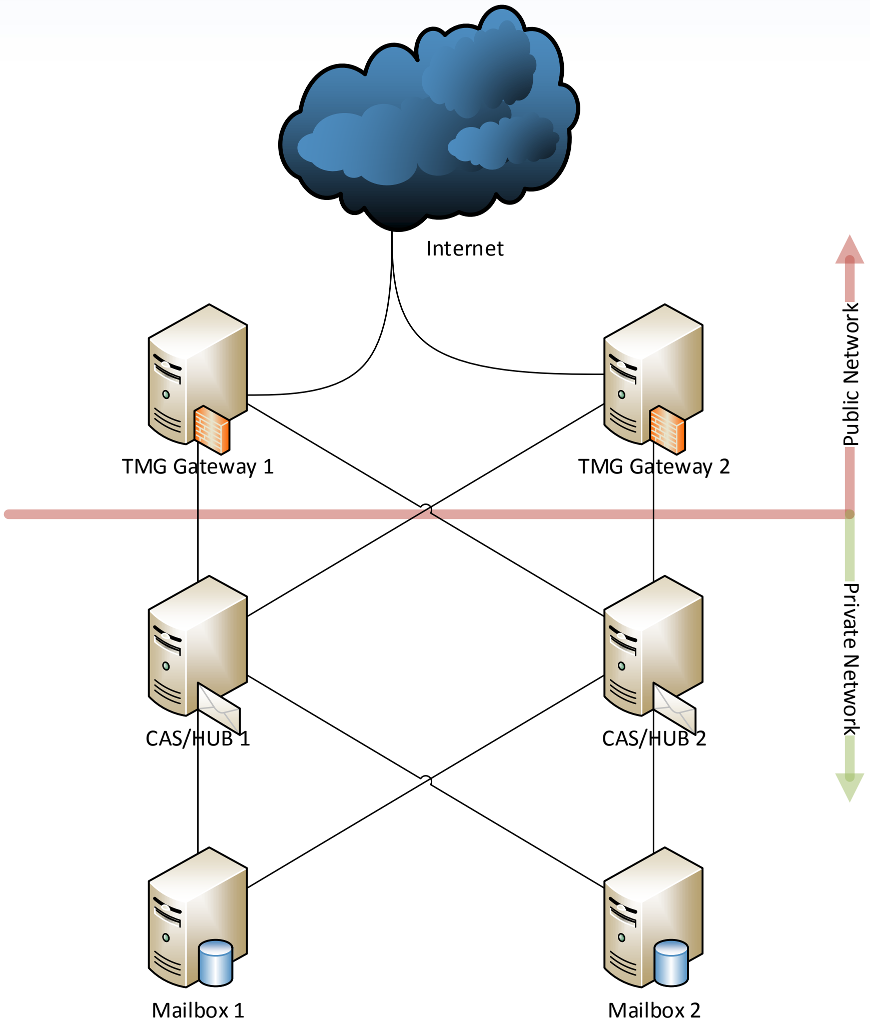
- More than 350 VMs in the server farm
- ACIS Core services such as:
  - AD controllers, LDAP, Exchange, Lync, Sharepoint
  - HA Clustered MSSQL, MySQL, PostgreSQL
  - DNS, DHCP, cluster login and service nodes
- Project based VMs
  - Software development, testing, code repos, continuous integration
  - iRODS servers, databases for iRODS catalog
  - ExoGENI has about 35 VMs, including
    - control.exogeni.net: exogeni's master ldap, puppet, and DNS
    - geni.renci.org: ORCA service manager which allows stitching vlans across racks
  - NetCDF data distribution
- We underestimated the value (demand)
  - Would prefer to have various levels of QOS, partition of services along differing SLA requirements

# VM Farm Example: Exchange e-mail services

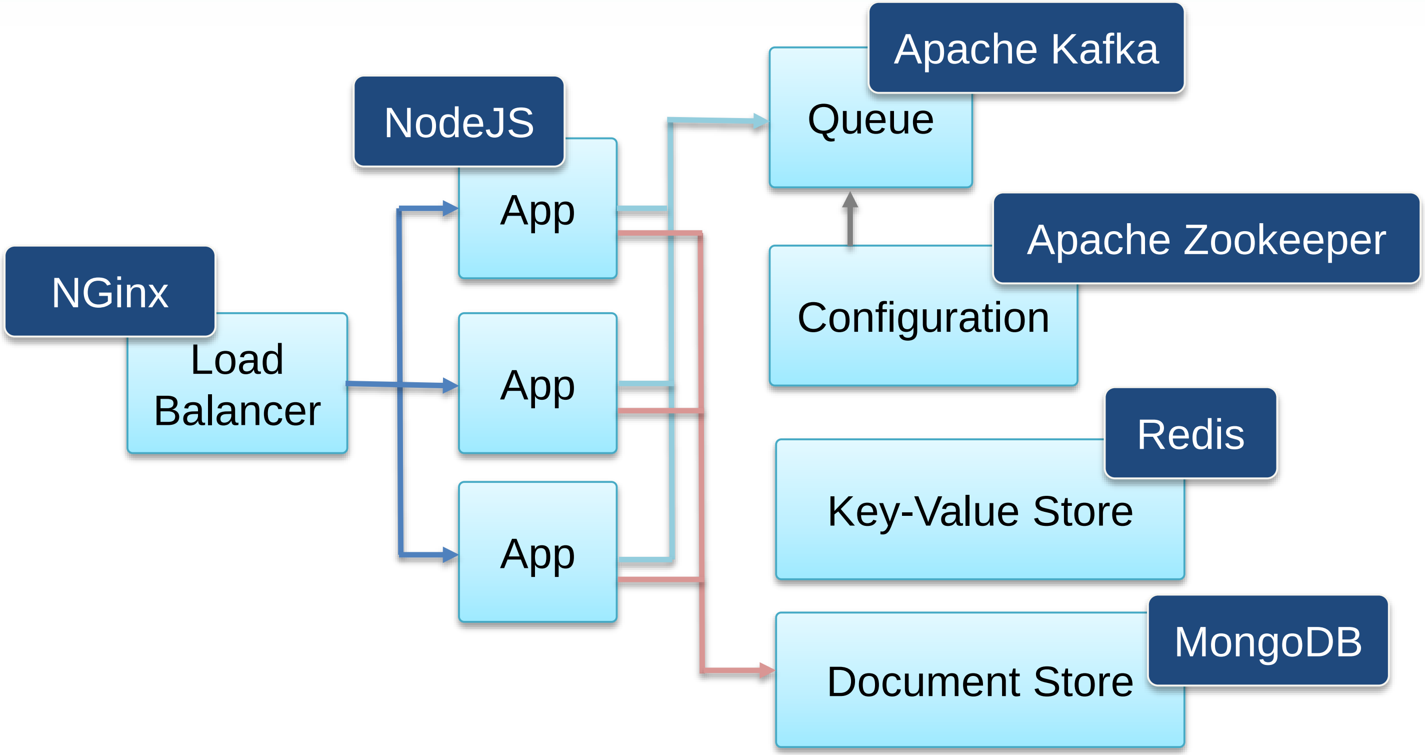
- 6 virtual machines to run the system

- We began hosting our own e-mail services before outsourcing was a viable option

- Community has grown accustomed to a level of service that can be difficult to achieve with the university central IT offerings, or commercial providers



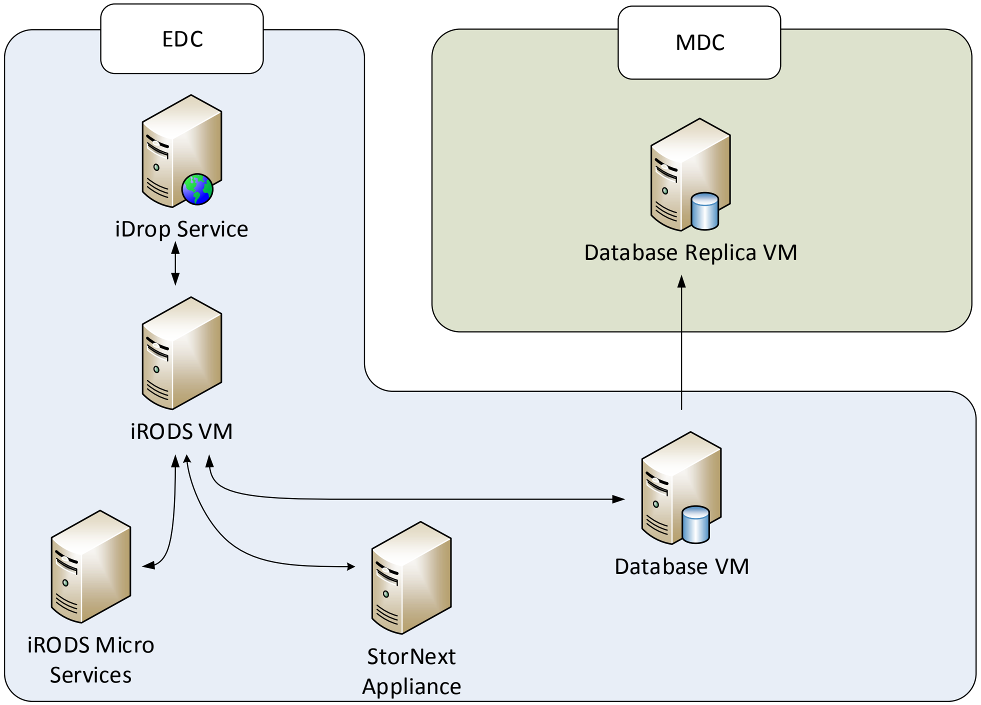
# VM Farm Example: Skylr – Distributed Alpha



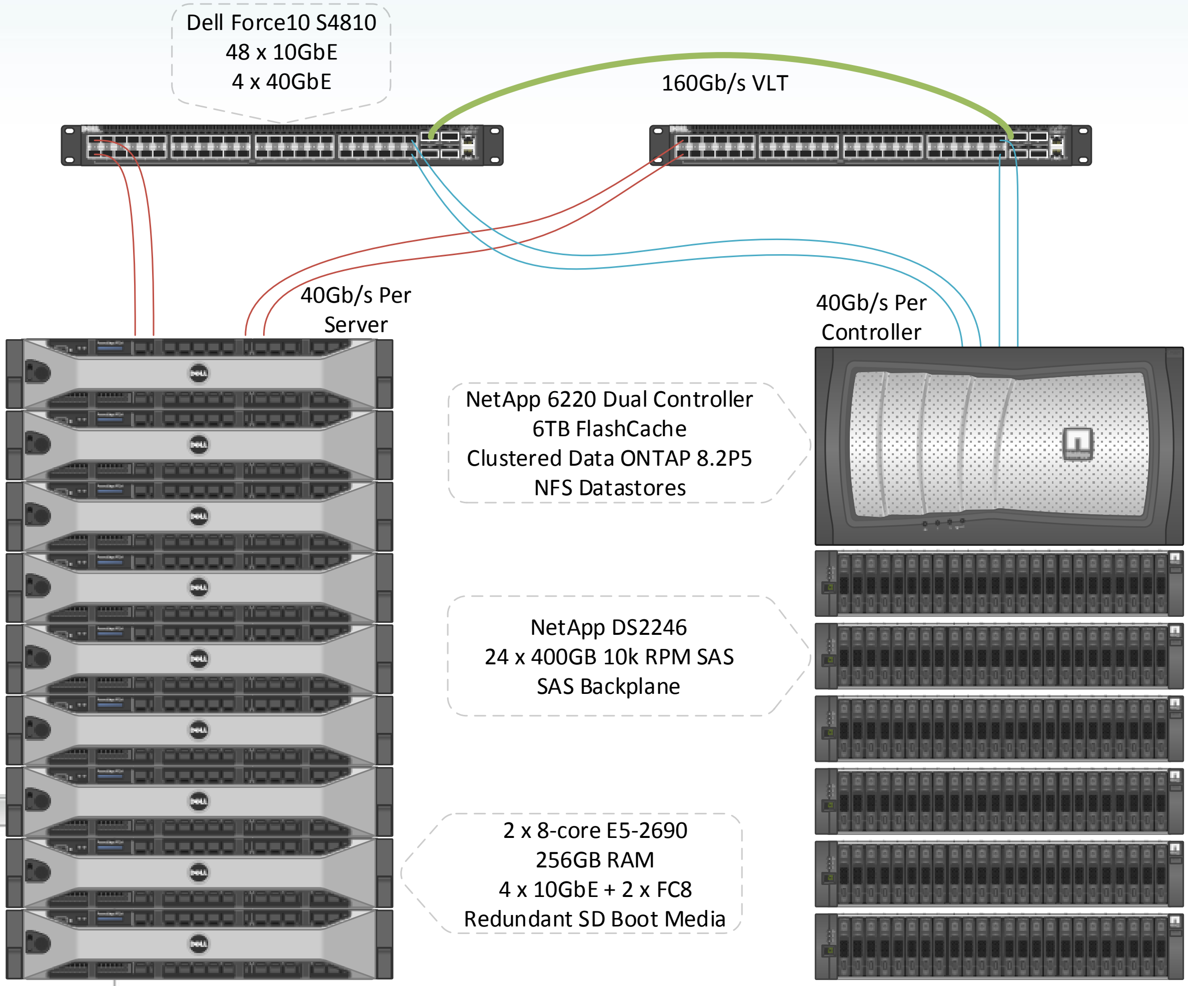
20 VMs total: two instances of this architecture, plus 4 dev/utility VMs

# VM Farm Example: Production iRODS deployment

- iren2.renci.org
- Multisite catalog replication
- Hydroshare microservices
- Serves the following data grids:
  - DFC
  - UNC Lifetime Library
  - CAMERA
  - TDLC



# Virtual Machine Services: VMWare



Dell Force10 S4810
48 x 10GbE
4 x 40GbE

160Gb/s VLT

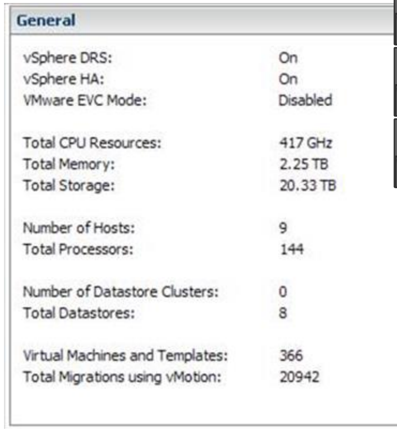
40Gb/s Per Server

40Gb/s Per Controller

NetApp 6220 Dual Controller
6TB FlashCache
Clustered Data ONTAP 8.2P5
NFS Datastores

NetApp DS2246
24 x 400GB 10k RPM SAS
SAS Backplane

2 x 8-core E5-2690
256GB RAM
4 x 10GbE + 2 x FC8
Redundant SD Boot Media



| General | |
|---|---|
| vSphere DRS: | On |
| vSphere HA: | On |
| VMware EVC Mode: | Disabled |
| Total CPU Resources: | 417 GHz |
| Total Memory: | 2.25 TB |
| Total Storage: | 20.33 TB |
| Number of Hosts: | 9 |
| Total Processors: | 144 |
| Number of Datastore Clusters: | 0 |
| Total Datastores: | 8 |
| Virtual Machines and Templates: | 366 |
| Total Migrations using vMotion: | 20942 |

Aggregate: 144 cores, 2.3TB RAM

# VM Farm: Just because we can, doesn’t mean we should …

We utilize external service providers wherever appropriate.
Websites on HostGator that we manage for more than 20 domains including:

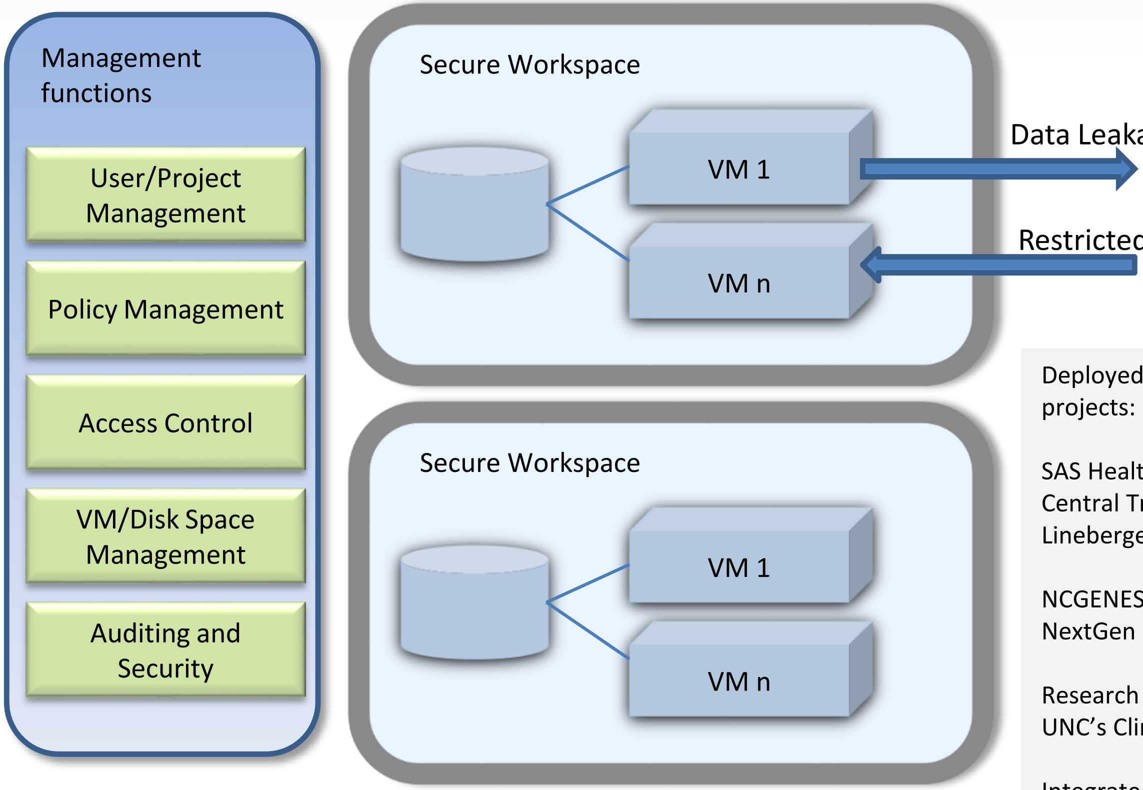
http://reachnc.org
http://coastalhazardscenter.org
http://mitigationguide.org
http://diph.renci.org
http://dice.renci.org
http://datafed.org
http://e-irods.org

http://ncdatascience.org
http://irods-consortium.org
http://www.ncgenes.org
http://www.exogeni.net
http://cuahsi.hydroshare.org
http://www.renci.org
. . .

RENCI web developer **Joe Hope** manages these in collaboration with our partners

# Secure Medical Workspace

## Managed Infrastructure



Data Leakage Protection (active filtering, DMZ,…)

Restricted access (firewall, VPN,…)

**A secure workspace consist of one or more virtual machines (VMs) that are provisioned along with a common data space to a research team. Multiple workspaces are controlled through a unified management system**

Deployed versions in different data-intensive research projects:

SAS Healthcare Analytics and the UNC Survivorship Cohort Central Tracking System, a collaboration between UNC’s Lineberger Comprehensive Cancer Center and SAS;

NCGENES (North Carolina Clinical Genomic Evaluation by NextGen Exome Sequencing) in the Department of Genetics;

Research on patient data sets governed by NC Tracs, holder of UNC’s Clinical and Translational Science Award

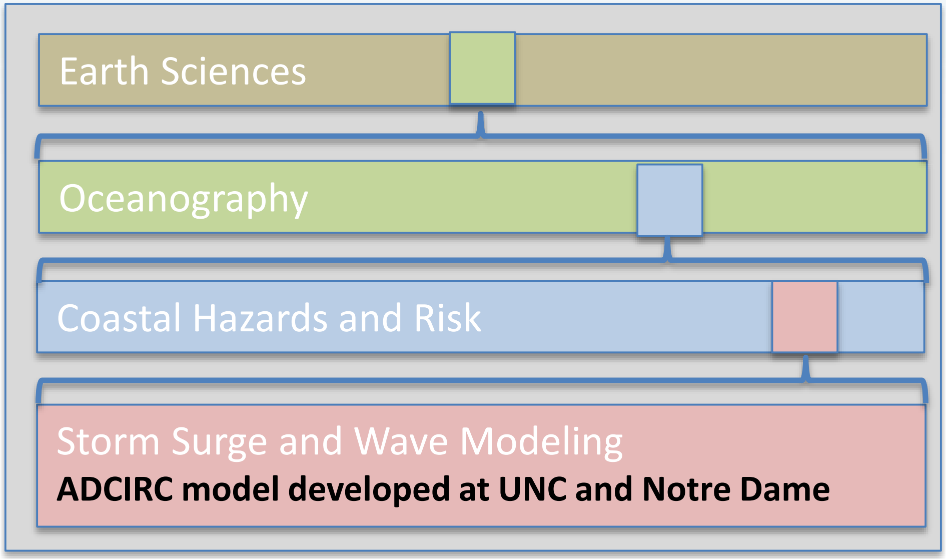
Integrated Cancer Information and Surveillance System at the Lineberger Comprehensive Cancer Center.

Evaluating the cost-effectiveness of the SMW for campus-wide adoption as a central component of its Information Security Plan following a comprehensive assessment of the technology.

**Contact: Charles Schmitt, RENCI**

http://www.ncbi.nlm.nih.gov/pubmed/23751029

# Environmental Sciences Program: Brian Blanton et al



Earth Sciences

Oceanography

Coastal Hazards and Risk

Storm Surge and Wave Modeling

**ADCIRC model developed at UNC and Notre Dame**

Funding sources

Public:

- NSF
- NOAA
- DHS & FEMA
- USACE
- NRC

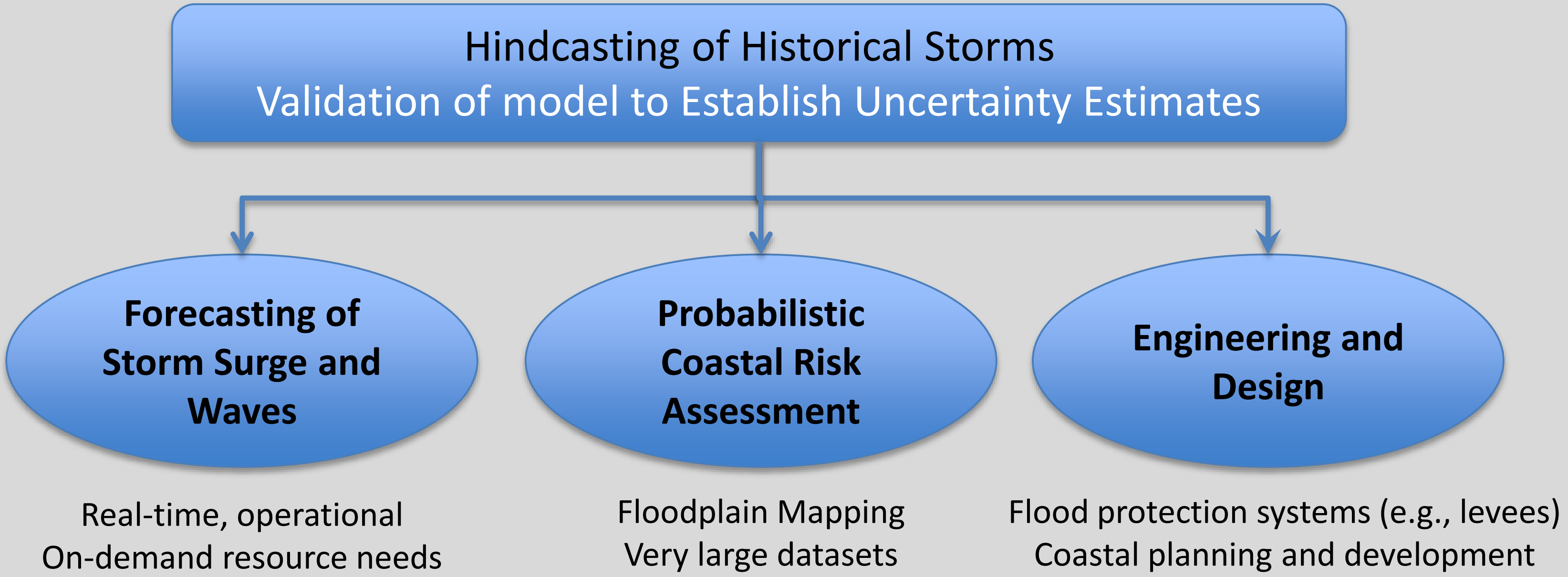
Private:

- Engineering Firms
- Utilities
- Commercial

Insurance

- Consulting

Research, Applications, and Operations with the ADCIRC storm surge, tide, and wave model



Hindcasting of Historical Storms
Validation of model to Establish Uncertainty Estimates

**Forecasting of Storm Surge and Waves**

Real-time, operational
On-demand resource needs

**Probabilistic Coastal Risk Assessment**

Floodplain Mapping
Very large datasets

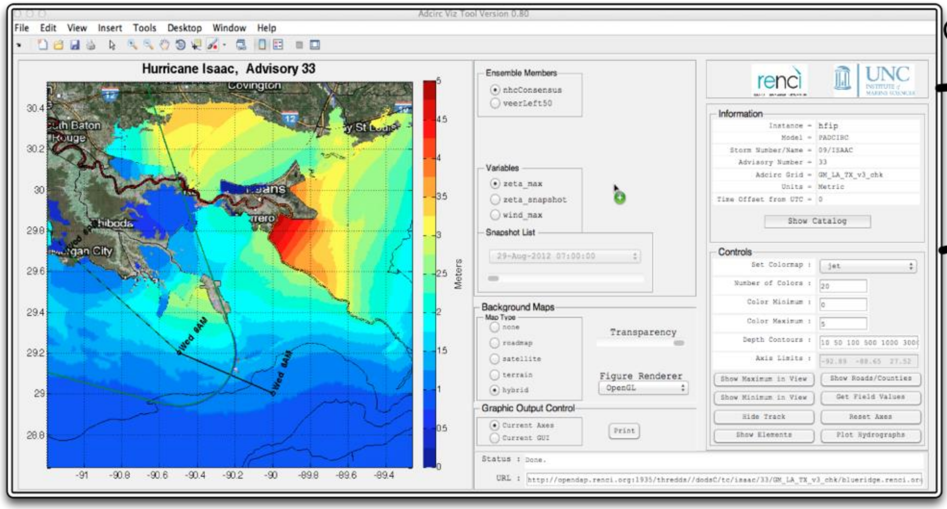
**Engineering and Design**

Flood protection systems (e.g., levees)
Coastal planning and development

# Coastal Hazards Community of Practice

AdcircViz during Hurricane Isaac (2012)

Collection of ADCIRC forecasting systems


Adcirc Viz Tool Version 0.80
File Edit View Insert Tools Desktop Window Help
Hurricane Isaac, Advisory 33
Covington
Baton Rouge
St Louis
Orleans
Thibodaux
Morgan City
Meters
renci
UNC Institute of Marine Sciences

Ensemble Members
● nhcConsensus
○ veerLeft50

Variables
● zeta_max
○ zeta_snapshot
○ wind_max

Snapshot List: 29-Aug-2012 07:00:00

Background Maps
Map Type
○ none
○ roadmap
○ satellite
○ terrain
● hybrid

Transparency

Figure Renderer: OpenGL

Graphic Output Control
● Current Axes
○ Current GUI

Print

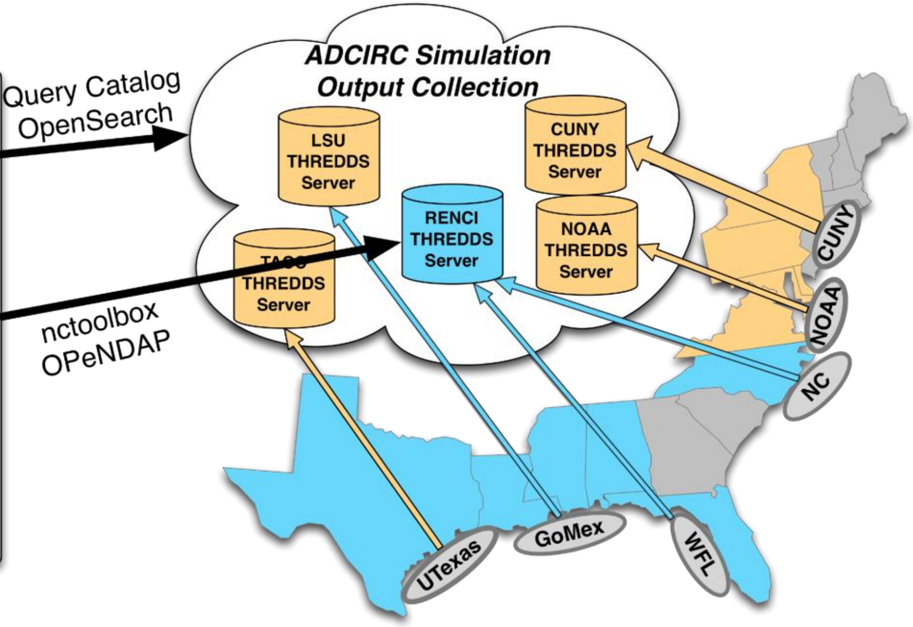
Information
Instance = hfip
Model = PADCIRC
Storm Number/Name = 09/ISAAC
Advisory Number = 33
Adcirc Grid = GM_LA_TX_v3_chk
Units = Metric
Time Offset from UTC = 0

Show Catalog

Controls
Set Colormap : jet
Number of Colors : 20
Color Minimum : 0
Color Maximum : 5
Depth Contours : 10 50 100 500 1000 300
Axis Limits : -92.89 -88.65 27.52

Show Maximum in View | Show Roads/Counties
Show Minimum in View | Get Field Values
Hide Track | Reset Axes
Show Elements | Plot Hydrographs

Status : Done.
URL : http://opendap.renci.org:1935/thredds//dodsC/tc/isaac/33/GM_LA_TX_v3_chk/blueridge.renci.or



Time sensitive ensemble HPC, as storms approach
Would benefit greatly from HPC resource sharing

http://people.renci.org/~bblanton/files/AdcircDuringIrene.key.pdf

# Some examples of Project Specific Hardware (PSH)

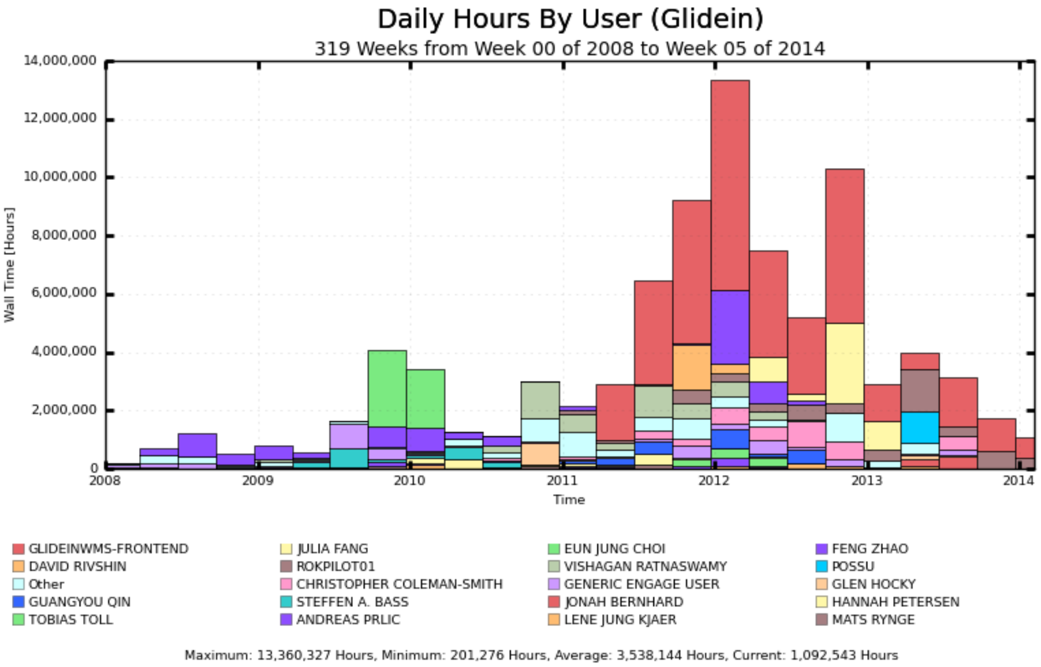
my apologies for the acronym, but too many letters otherwise

# PSH: OSG EngageVO

- Assisting researchers with access to OSG since 2007

- engage-submit3.renci.org, physical machine
- 30 TB disk mounted to the submit host (re-purposed out of warranty)
- VMs for associated services (eg VOMS)

- RENCI Identity management for access to submit host, OSG credentials from there
- Newer methods available now: OSG Connect



# PSH: Relational Database for Genomics

- Essentially a Croatan node
  - Dell R720xd, 256GB ram
  - 32TB DAS:  12 x 3TB NLSAS
  - Runs MS SQL Server

  - Supports genomics work of Dr. Kirk Wilhelmsen
  - Several Databases that are many TBs in size, with billions of rows
  - Very heavily loaded system

# PSH: Coastal Emergency Risks Assessment, NC-CERA

- Visualize results of ensemble based HPC model runs
- Generates and serves map tile sets
- Tens of millions of small files generated regularly
- Storage latency is more important than throughput
- One small piece of the overall solution is an old c++ opengl code for Windows, and is a bottleneck which is driving hardware decisions

- Currently running on multiple blade servers with DAS from the out of warranty DDN equipment, planned upgrade to R720xd

http://nc-cera.renci.org/cera/_docs/CERA_NC_tutorial2013.pdf

http://www.ecu.edu/renci/_docs/2012HurricaneWorkshop/Blanton.pdf

# MDC: Manning Data Center; UNC Central IT

- 11,000-square-foot data center;
- In partnership with UNC Research Computing
- We wish to bridge the capabilities of these two University assets (EDC, MDC) and facilitate research that moves between them, enabling cross site redundancy and building a culture of shared distributed systems.

- Genomics and medical informatics are the primary use cases thus far
- DR for EDC research and production storage tiers
- A few project specific servers

- RENCI has a few racks here
- Small VM Farm
- 1.5 PB raw storage

# The Duke Social Computing Room (SCR)

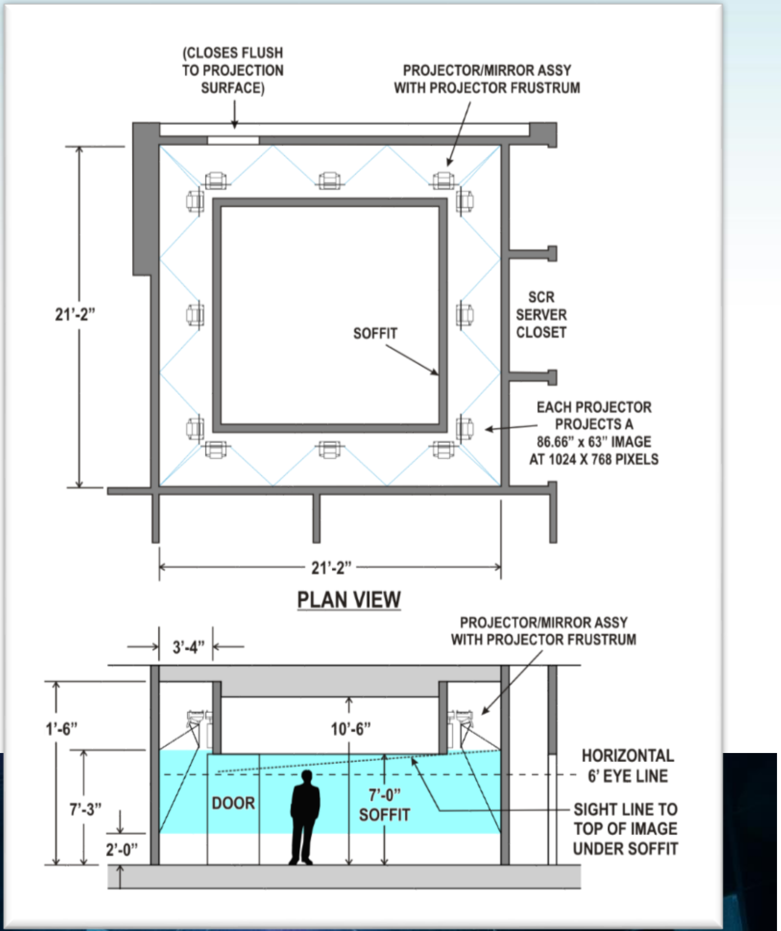
## In Development

**Currently deployed at RENCI's Engagement Center at UNC-Chapel Hill and NCSU, the SCR is …**

- A collaborative visualization environment for researchers and students that provides a large physical real estate for arranging visual information[1]
- A Windows 7-based display that consists of a square room with 12 projectors (3 per wall) used to display a single 360-degree desktop environment spanning all four walls
- A tool to visualize and explore large amounts of heterogeneous data
- A user-friendly environment that has a low barrier to entry

**In the SCR you can …**

- Boost presentations to a new level
- Conduct classes and seminars while surrounded by images, documents, movies, and visualizations
- Visualize and explore large data and documents
- Collaboratively develop grants, review code, and analyze large images, maps, and engineering documents
- Host videoconferences immersed in virtual worlds
- Develop innovative media installations



(CLOSES FLUSH TO PROJECTION SURFACE)
PROJECTOR/MIRROR ASSY WITH PROJECTOR FRUSTRUM
21'-2"
SOFFIT
SCR SERVER CLOSET
EACH PROJECTOR PROJECTS A 86.66" x 63" IMAGE AT 1024 X 768 PIXELS
21'-2"
PLAN VIEW
3'-4"
PROJECTOR/MIRROR ASSY WITH PROJECTOR FRUSTRUM
1'-6"
10'-6"
HORIZONTAL 6' EYE LINE
7'-3"
DOOR
7'-0" SOFFIT
SIGHT LINE TO TOP OF IMAGE UNDER SOFFIT
2'-0"

renci RESEARCH \ ENGAGEMENT \ INNOVATION

# SCR Applications:  Scientific Visualization

"The Social Computing Room is an ideal location to perform the design reviews and voting for the visualization homeworks in the Visualization in the Sciences class. We can project the entries from each student on the walls all **at the same time**, along with a text description of what questions they were supposed to answer, and then **all sit and talk about the comparative strengths and weaknesses** of each approach. The ability to **walk right up to the images** lets us both see them at **high detail** and vote (by dropping pennies) for our favorite visualizations. The central seating area makes the **room comfortable for hour-long sessions and extended discussions**. The USB input lets us bring our own content to be displayed. The **auto-layout software** combined with the **ability to move images** around manually enables us to **rapidly set up a session**."

– Russ Taylor, UNC-CH CS

Multiple model runs

Time-series data

# SCR Applications:  Research Meetings

- Melanoma Image Analysis
  - Segmentation and feature extraction of stained biopsy slides
  - Lots of data
    - Original images
    - Feature images
    - Feature distribution scatter plots
  - Ability to spread data out extremely helpful
  - Used weekly

Matlab tool for sorting images based on feature strength

# SCR Applications:  Arts and Humanities

Spectacular Justice

Multimedia art installation by Joyce Rudinsky

Part of Carolina Performing Arts
*Criminal/Justice: The Death Penalty Examined*

Images, video, and audio respond to user locations

Extensions for this project:

- Ubisense tracking system
- 2 HoloPro rear-projection screens w/ auxiliary projectors
- 5 Directional speakers
- PosiTrack camera controller

# SCR Take Home

- Easy to use
  - Single PC
  - Run practically any existing software
  - Standard interface
- Customizable
  - Hardware + software
  - Coding in general…
- Collaborative
  - Multiple people
  - Currently only single point of control…

# GSB: Genome Sciences Building

TopSail: decommissioned from UNC ITS Research Computing, managed by Erik Scott

- 400 nodes, 3200 cores
- 400x1.5T (600 T) disk + 108 TB scratch
- 400 gbits/sec of usable Hadoop bandwidth

- 4 or 8 cores per disk drive
- 2 gigabit campus connectivity to datamover – less than 1 gb/s to Renci

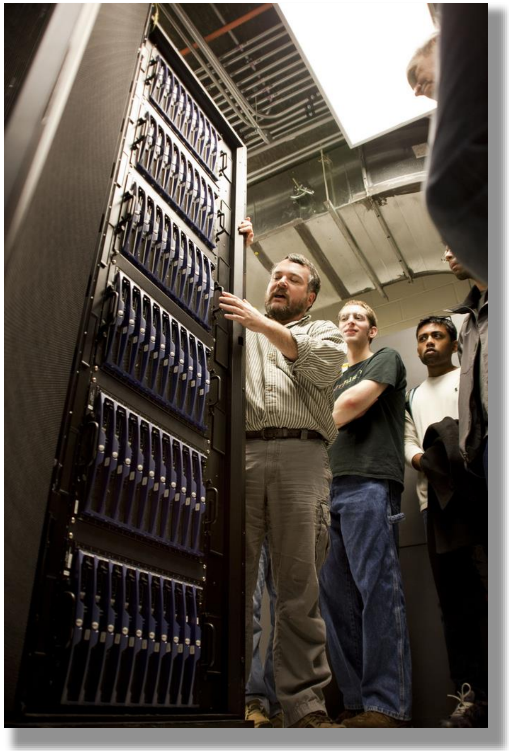
- Apache Hadoop w/ Pig, Hive, Mahout, Zookeeper
- DB/2 parallel query edition
- HDFS FUSE Bridge on datamover
- Backups (slowly!) to RENCI tape

# The National Consortium for Data Science

UNC Chapel Hill: Computer Science 790-042
*Data Center Systems and Programming* Prof. Don Smith

- One of the NCDS focus areas: Workforce Development

- Graduate Seminar on Large-Scale Computing Methods and Issues
- Key topics: Storage, Networking, Computing, Power and Cooling
- Basic introduction to Hadoop through directed readings and two Hadoop-based projects
- ~15 graduate students



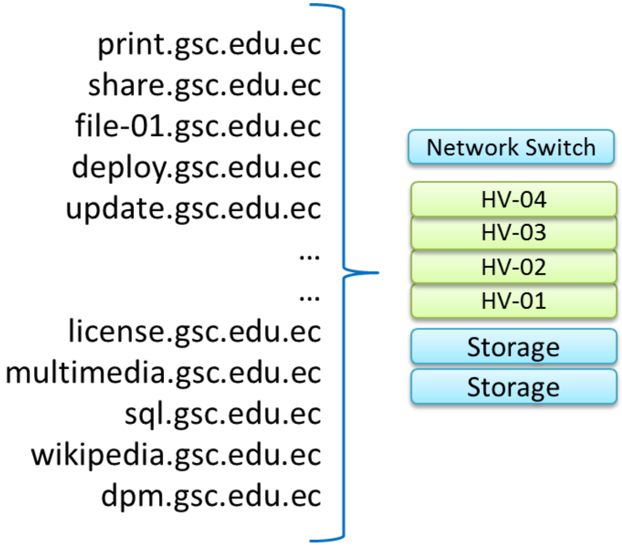
Erik Scott

**www.data2discovery.org**

http://data2discovery.org/dev/wp-content/uploads/2014/02/NCDS-Summit-2013.pdf

# GSC: Galapagos Science Center

- Remote Branch Office Scenario
- Extreme network limitations
- Supports Center operations and onsite research and teaching activity
- GIS Lab with approx. 15 workstations
- UNC and USFQ Campus Identity Management extended to the facility
- MSFT Hyper-V



print.gsc.edu.ec
share.gsc.edu.ec
file-01.gsc.edu.ec
deploy.gsc.edu.ec
update.gsc.edu.ec
…
…
license.gsc.edu.ec
multimedia.gsc.edu.ec
sql.gsc.edu.ec
wikipedia.gsc.edu.ec
dpm.gsc.edu.ec

Network Switch
HV-04
HV-03
HV-02
HV-01
Storage
Storage

# Directory Services and Identity Management

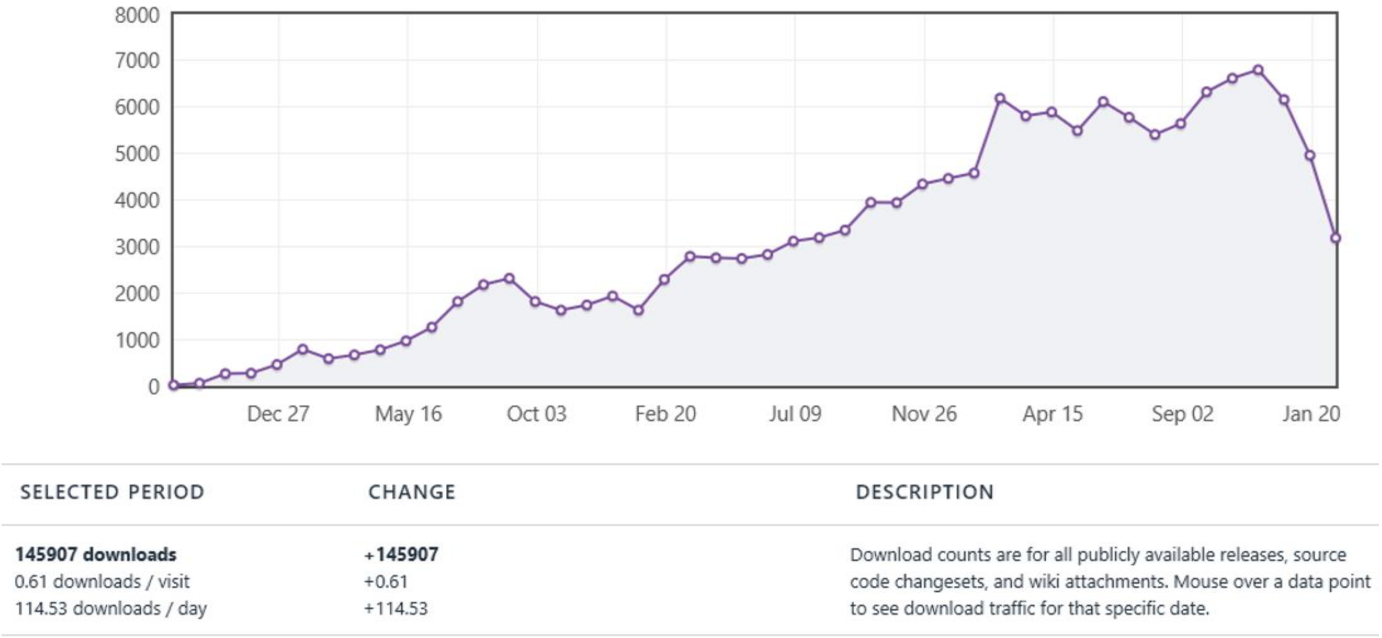
- LDAP and Active Directory
- There are 12 times as many external collaborators in the directory as there are RENCI staff
- Consolidating on Active Directory, eliminating LDAP
- Cluster nodes are now using SSSD vs distributed passwd files
- Shibboleth is used in some cases (eg REACH-NC)
- iRODS based projects federated at the iRODS layer
- ExoGENI project maintains their own LDAP
- We wish to federate with UNC or adopt UNC credentials for institute staff, while maintaining a directory for external collaborators
- Very difficult to acquire the required time and service interruptions for a more appropriate solution

# And a few things we did not talk about …

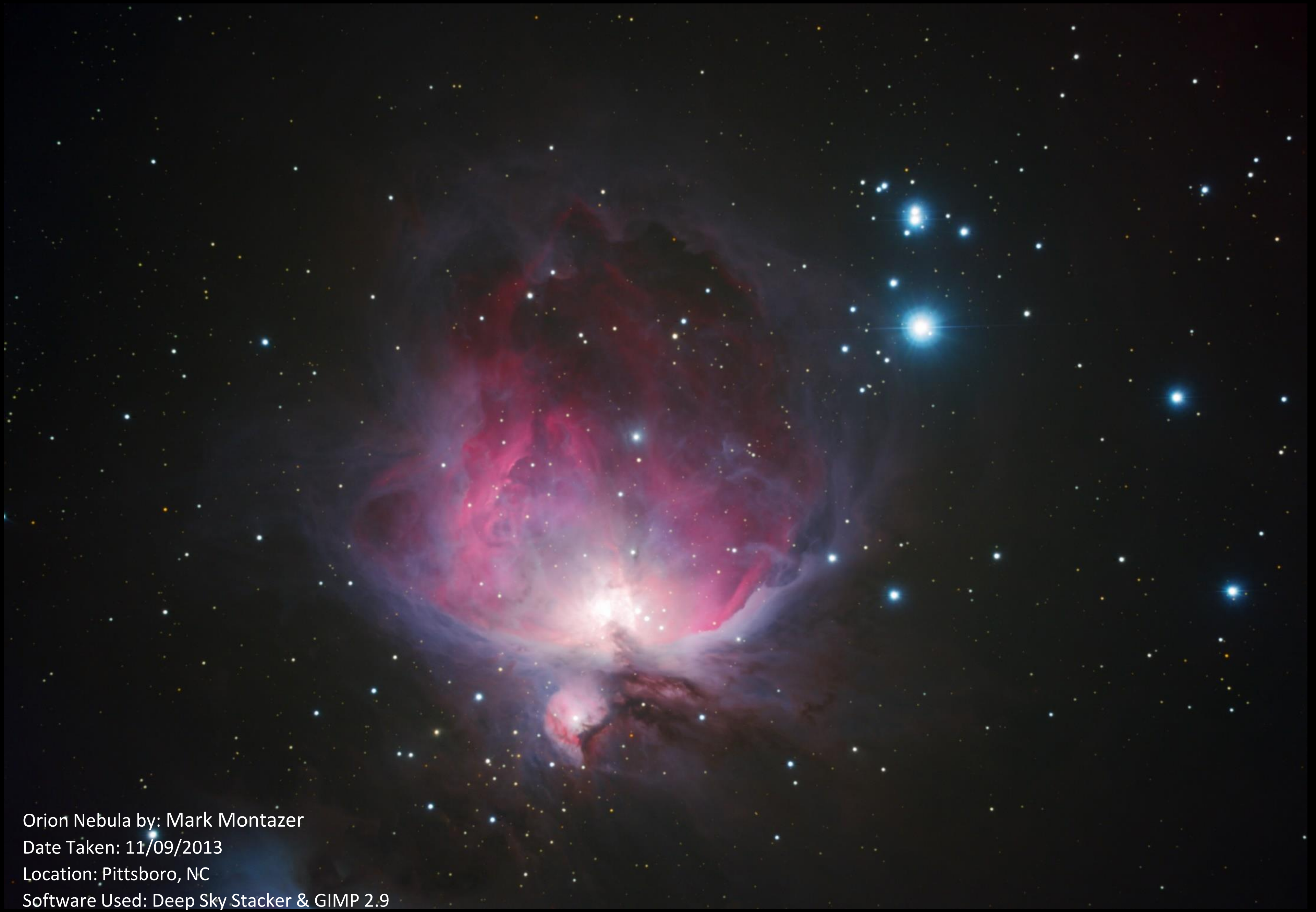
- Monitoring and notification: nagios, snmp, SCOM
- PXE boot: laptops, VMs, cluster nodes
- DNS, DHCP, VPN
- CommVault Backup
- HA Clustered relational databases
- FTP/HTTP servers and frameworks (PHP, Tomcat, etc.)
- Dell Open Manage Essentials
- Multisite data replication: block level, file level
- Compiler support: GNU gcc/gfortran, Intel icc/ifort and Portland Group (PGI) pgcc/pgfortran
- MPI Support: mvapich, openmpi and intel MPI
- Configure, compile and install: NetCDF, HDF, Nvidia CUDA, Intel MIC platform, hpctoolkit
- Manage licenses for Matlab, Intel and PGI compilers
- Special Engagements, eg experimental replacement for TCP, deployed at endpoints between EDC and MDC; Prof. Don Smith, UNC-CS

# SSH.NET – .NET native open source SSH

- Open source .NET library for building solutions with SSH capabilities
- Makes use of advanced features of the Microsoft platform
- More than: 145k downloads, 1M page views
- Active discussion boards
- [http://sshnet.codeplex.com](http://sshnet.codeplex.com)



| SELECTED PERIOD | CHANGE | DESCRIPTION |
|---|---|---|
| **145907 downloads**<br>0.61 downloads / visit<br>114.53 downloads / day | **+145907**<br>+0.61<br>+114.53 | Download counts are for all publicly available releases, source code changesets, and wiki attachments. Mouse over a data point to see download traffic for that specific date. |



Orion Nebula by: Mark Montazer
Date Taken: 11/09/2013
Location: Pittsboro, NC
Software Used: Deep Sky Stacker & GIMP 2.9
30 3-minute exposures at ISO 800, 30 2-minute exposures at ISO 800, 40 20-second exposures at ISO 800 for a 2-hour & 43-minute integrated exposure
Equipment: Sony NEX-5 (modified for astrophotography) using a 731mm f/4.8 Maksutov-Newtonian telescope on a Celestron CG5-ASGT mount

# END PRESENTATION

renci

RESEARCH \ ENGAGEMENT \ INNOVATION